ZnO Nanostructures: A Heterogeneous Catalyst for the Synthesis of Benzoxanthene and Pyranopyrazole scaffolds via multi-component reaction strategy

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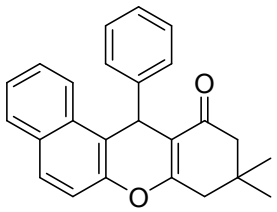
Supporting Information

Table S1

Sr. No.	Product	Characterization
1		Entry 4a: 9, 9-Dimethyl-12-phenyl-8, 9, 10, 12-tetrahydro-benzo[a]xanthenes-11-one: ^{1}H NMR (300 MHz, DMSOd_6): δH ppm 7.1-8.4 (m, 11H, ArH), 5.3 (s, 1H, CH), 2.6 (s, 2H, CH_2), 2.2-2.4 (m, 2H, CH_2), 1.1 (s, 3H, CH_3), 0.96 (s, 3H, CH_3). ^{13}C NMR (75MHz, DMSO): δ ppm 196.78, 162.61, 148.68, 144.32, 130.32, 130.16, 128.52, 128.16, 126.38, 124.45, 124.16, 117.36, 116.52, 114.22, 50.65, 40.36, 33.87, 32.52, 29.28, LCMS: m/z = 377.14

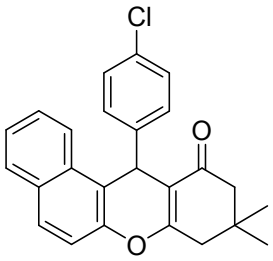
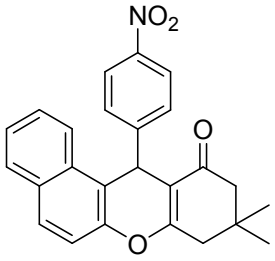
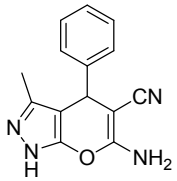
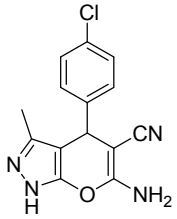
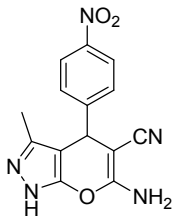
2		Entry 4b: 9, 9-Dimethyl-12-(4-chlorophenyl)-8, 9, 10, 12-tetrahydro-benzo[a]xanthenes11-one: ^{1}H NMR (300 MHz, $DMSOd_6$): δH ppm 7-7.9 (m, 10H, ArH), 5.72 (s, 1H, CH), 2.6 (s, 2H, CH_2), 2.2-2.4 (m, 2H, CH_2), 1.2 (s, 3H, CH_3), 0.098 (s, 3H, CH_3). ^{13}C NMR (75MHz, DMSO): δ ppm 196.44, 164.47, 147.61, 144.29, 131.57, 131.24, 130.97, 130.47, 129.84, 129.08, 128.61, 127.75, 125.56, 123.70, 117.65, 117.17, 113.25, 50.54, 40.68, 39.98, 34.06, 29.26, 26.71. LCMS: m/z =
3		Entry 4c: 9, 9-Dimethyl-12-(4-nitrophenyl)-8, 9, 10, 12-tetrahydro-benzo[a]xanthenes-11- one: ^{1}H NMR (300 MHz, $DMSOd_6$): δH ppm 7.3-7.4 (m, 10H, ArH), 5.6 (s, 1H, CH), 2.7 (s, 2H, CH_2), 2.1-2.2 (m, 2H, CH_2), 1.2 (s, 3H, CH_3), 0.98 (s, 3H, CH_3). ^{13}C NMR (75MHz, DMSO): δ ppm 196.80, 164.57, 151.47, 147.65, 146.36, 131.45, 131.13, 129.84, 128.56, 127.35, 123.61, 123.21, 117.15, 113.20, 50.59, 41.36, 34.68, 29.48, 27.16. LCMS: m/z =

Table S2

Entry	Product	Characterization
1		Entry5a:6-Amino-5-cyano-3-methyl-4-phenyl-2H,4H-dihydropyrano[2,3-c]pyrazole: ^{1}H NMR (400 MHz, DMSO-d_6): = 12.20 (s, 1H), 7.20 (d, 2H), 7.20 (d, 2H), 6.98 (s, 2H), 4.80 (s, 1H), 1.98 (s, 3H) ppm ^{13}C NMR (100 MHz, DMSO-d_6): = 160.8, 154.7, 144.3, 135.5, 128.3, 127.3, 126.6, 120.6, 97.6, 57.3, 36.2, 9.6 ppm, LCMS: m/z: 253.1, found: 253.2;
2		Entry 5b: 6-Amino-4-(4-chlorophenyl)-5-cyano-3-methyl-2H, 4H-dihydropyrano[2,3-c]pyrazole: ^{1}H NMR (400 MHz, DMSO-d_6): = 12.20 (s, 1H), 7.98 (d, 2H, J = 8.3 Hz), 6.98 (d, 2H, J = 8.3 Hz), 6.98 (s, 2H), 4.80 (s, 1H), 1.98 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6): = 165.76, 161.38, 158.91, 157.47, 155.17, 144.45, 143.97, 130.14, 131.81, 129.84, 128.90, 121.13, 120.05, 97.66 ppm, LCMS: m/z
3		Entry 5c: 6-Amino-5-cyano-3-methyl-4-(4-nitrophenyl)-2H,4H-dihydropyrano[2,3-c] ^{1}H NMR (400 MHz, DMSO-d_6): = 12.24 (s, 1H), 7.98(d, 2H, J = 8.4 Hz), 7.68 (d, 2H, J = 8.4 Hz), 6.98 (s, 2H), 4.82 (s, 1H), 1.91 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6): = 164.16, 160.84, 157.94, 154.86, 152.36, 145.53, 135.8, 129.67, 128.70, 120.3, 96.65 ppm, LCMS:m/z

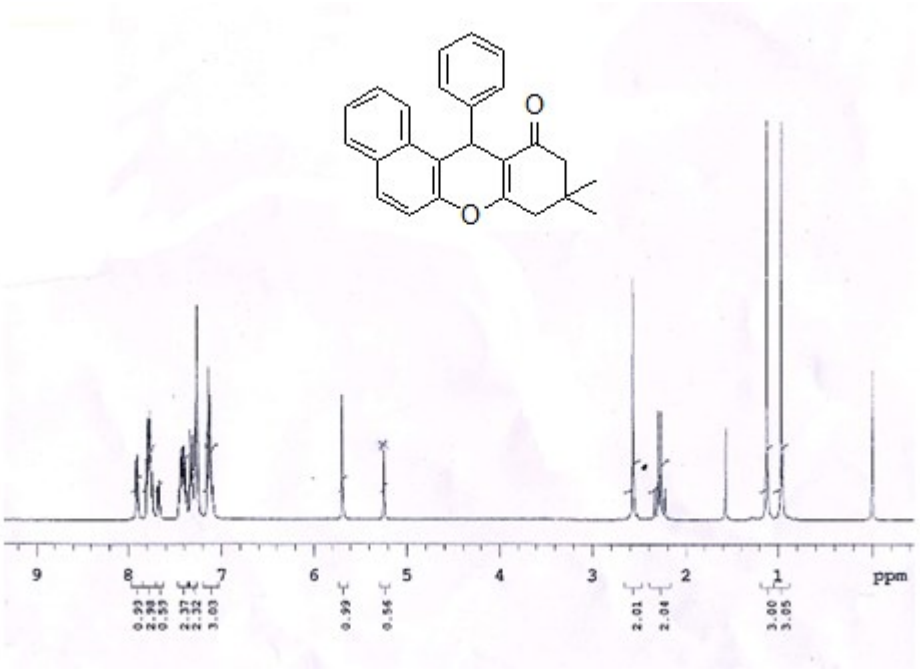


Fig. S1 ^{1}H NMR spectrum of 9, 9-Dimethyl-12-phenyl-8, 9, 10, 12-tetrahydro-benzo[a]xanthenes-11-one:

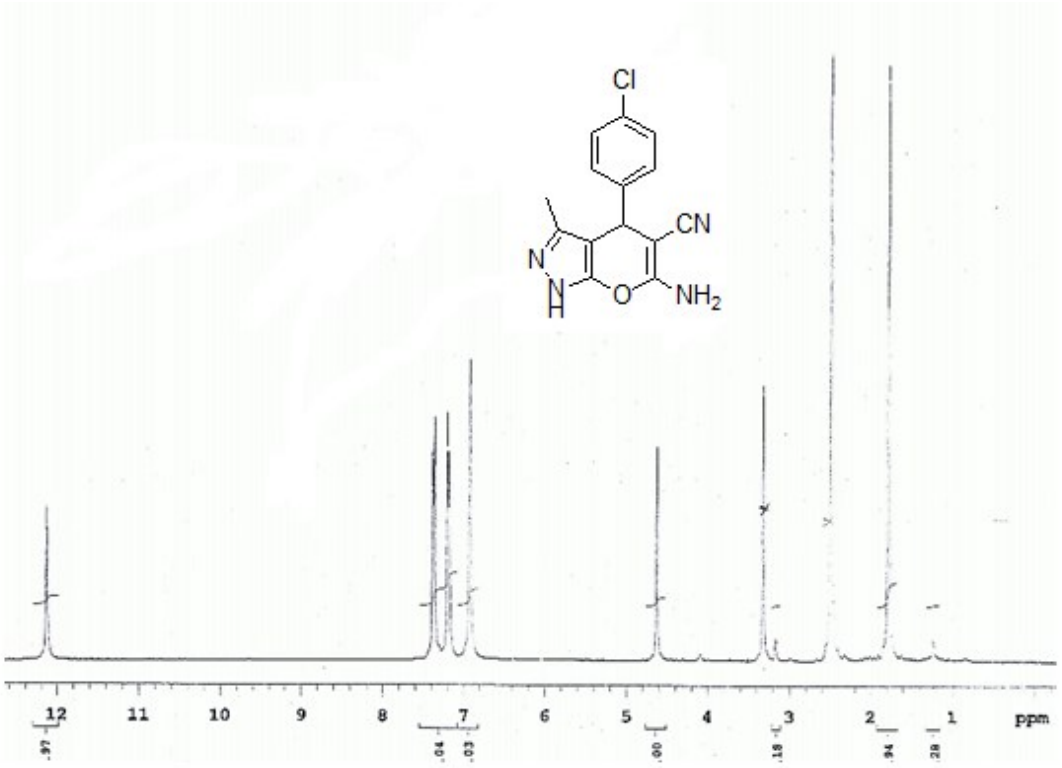


Fig.S2[1]H NMR spectrum of 6-Amino-4-(4-chlorophenyl)-5-cyano-3-methyl-2H, 4H-dihydropyrano[2,3-c]pyrazole

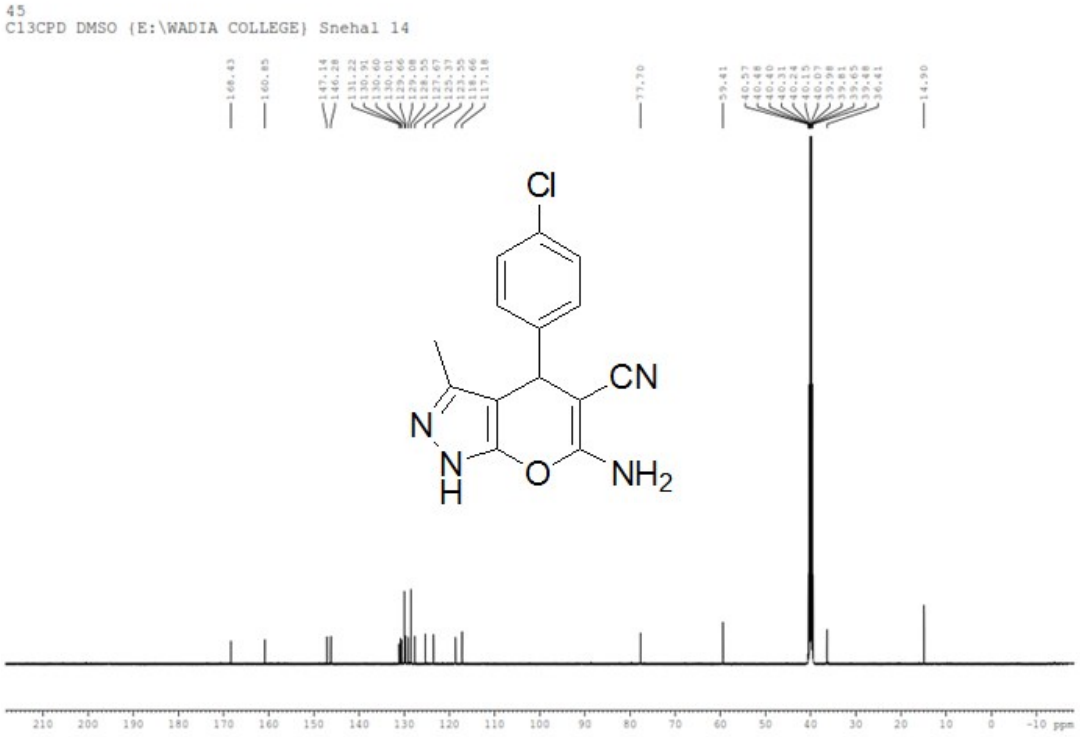
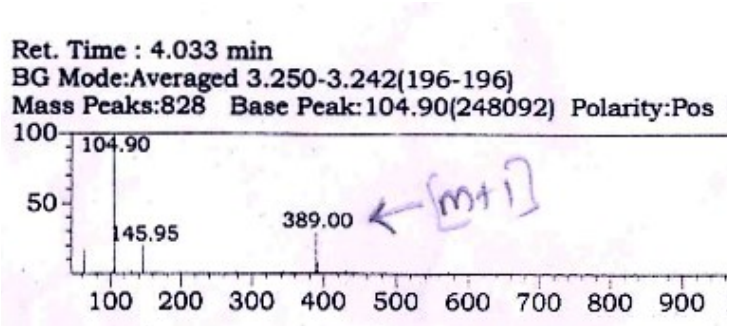


Fig. S3^{13}C NMR spectrum of 6-Amino-4-(4-chlorophenyl)-5-cyano-3-methyl-2H, 4H-dihydropyrano[2,3-c]pyrazole

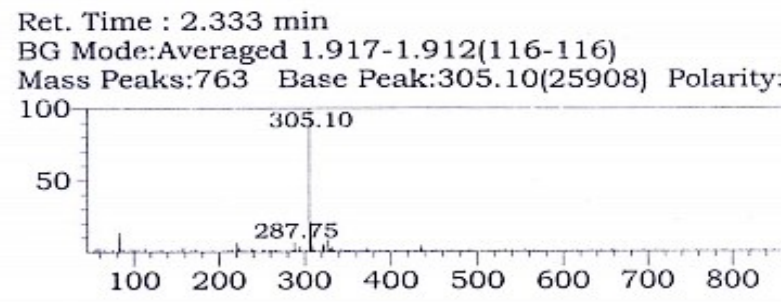
Fig.S4^{13}C NMR spectrum of 9, 9-Dimethyl-12-(4-chlorophenyl)-8, 9, 10, 12-tetrahydro-benzo[a]xanthenes11-one

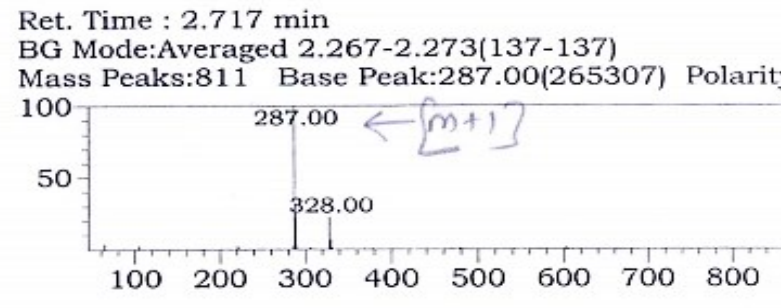


PeakTable
PDA Ch1 210nm - 400nm 4nm

Peak#	Ret. Time	Area	Area %
1	2.843	1151283	15.995
2	2.923	17928	0.249
3	3.659	27733	0.385
4	3.978	6000838	83.371
Total		7197781	100.000

Fig. S5.15 LCMS of 9, 9-Dimethyl-12-(4-chlorophenyl)-8, 9, 10, 12-tetrahydro-benzo[a]xanthenes11-one





PeakTable
PDA Ch1 210nm - 400nm 4nm

Peak#	Ret. Time	Area	Area %
1	2.164	22582	0.134
2	2.215	42548	0.253
3	2.301	82117	0.489
4	2.421	14665	0.087
5	2.467	22439	0.134
6	2.589	12137	0.072
7	2.677	16550117	98.545
8	3.100	4356	0.026
9	3.178	43593	0.260
Total		16794553	100.000

Fig. S6 6-Amino-4-(4-chlorophenyl)-5-cyano-3-methyl-2H, 4H-dihydropyrano[2,3-c]pyrazole

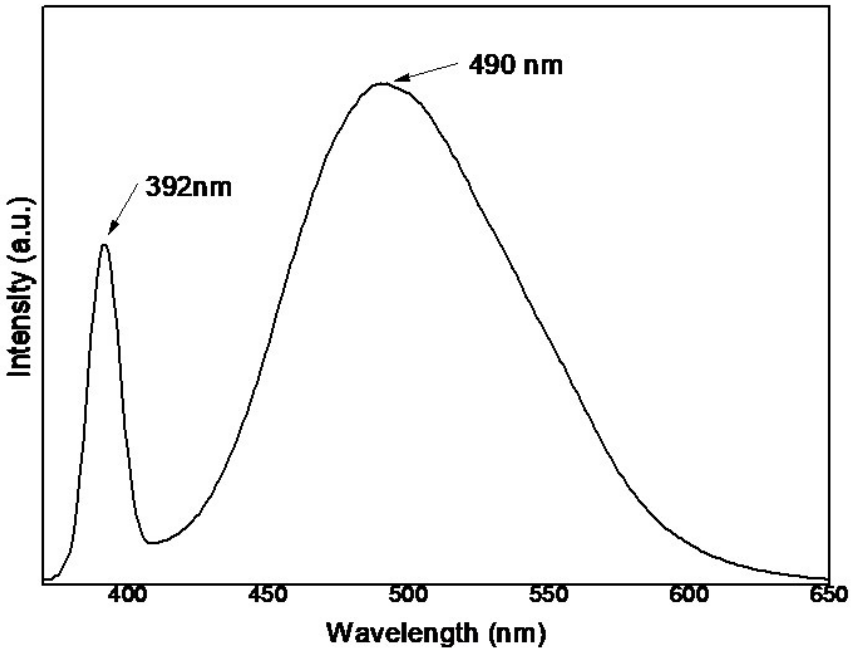


Fig. S7 Photoluminescence spectra of ZnO nanostructure at excitation wavelength 350 nm